A Molecular Model for Engineering Applications: Phase Behavior, Interfacial Properties, and Microstructure of Complex Fluids

Walter G. Chapman, W.W. Akers Chair Professor, Chemical and Biomolecular Engineering Dept., Rice University

To design and optimize processes and products in the energy, chemicals, and materials industries, engineers need computational tools to predict bulk and interfacial equilibrium properties for complex fluids in terms of temperature, pressure, composition, and molecular geometry. Systems that have been particularly challenging to model include associating or polar molecules as well as polymers and amphiphiles. Past approaches in the industry have required specialized thermodynamic models for varying conditions and for each separate phase with sometimes unsatisfactory results.

Advances in statistical mechanics, such as the statistical associating fluid theory (SAFT), have led to successful molecular models for bulk fluids of associating and polyatomic molecules. SAFT enables engineers to predict the effects of molecular weight, polydispersity, polarity, association, and compressibility on the bulk phase behavior of mixtures containing solvents, monomers, polymers, and patchy colloids. Extensions using density functional theory have shown success in modeling interfacial properties and molecular structure, including the behavior of fluids at hydrophilic and hydrophobic surfaces, segregation in polymer blends and polymer/colloid systems, and self-assembly of surfactants and block copolymers.

In this presentation, the physical basis of the SAFT approach will be described and insights into the behavior of fluids will be discussed based on applications in the upstream and downstream. Examples will include phase behavior in mixtures of molecules with large size asymmetry, water content in hydrocarbons, and interfacial behavior and self-assembly of amphiphilic molecules.